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Nanofiltration performance of conical and hourglass nanopores

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Abstract

Pressure-driven ion transport through conical and hourglass-shape (double conical) nanopores is investigated theoretically by solving the Poisson, Nernst-Planck and Navier-Stokes equations numerically. Due to the electrostatic asymmetry in conical nanopores, these latter exhibit nanofiltration rectification properties, i.e. they reject salts differently depending if the solution enters the nanopore from its base or its tip. The filtration rectification properties of conical nanopores result from two different phenomena, (i) the co-ion exclusion at the pore mouth and (ii) the sign and the magnitude of the (pressure-induced) electric field arising through the nanopores. Hourglass-shape nanopores exhibit improved separation performance compared with cylindrical and conical nanopores with identical average diameter, length and surface charge density. Notably, they allow target salt rejections to be reached with a smaller driving force than the other pore geometries, which makes them attractive candidates for the design of advanced nanofiltration membranes allowing less energy intensive separations.